A model for the structure of the hydrated aluminum phosphate, kingite determined by ab initio powder diffraction methods

KIA S. WALLWORK,[1] ALLAN PRING,[*,1,2,3] MAX R. TAYLOR,[1] AND BRETT A. HUNTER[4]

[1]School of Chemistry, Physics and Earth Sciences, The Flinders University of South Australia, GPO Box 2100 Adelaide, South Australia 5001, Australia
[2]Department of Mineralogy, South Australian Museum, North Terrace, Adelaide, South Australia 5000, Australia
[3]Department of Geology and Geophysics, Adelaide University, North Terrace, Adelaide, South Australia 5000, Australia
[4]Neutron Scattering Group, ANSTO, PMB 1, Menai, New South Wales 2234, Australia

ABSTRACT

The crystal structure of kingite, $Al_3(PO_4)_2(F,OH)_2 \cdot 8(H_2O,OH)$, a secondary mineral from a Cambrian-Precambrian phosphate deposit at Tom's Quarry, near Kapunda, South Australia, has been determined from a powder sample using synchrotron X-ray diffraction data. The structure was determined ab initio by direct methods and refined to $R_{Bragg} = 0.022$ and $R_{wp} = 0.039$ using the Rietveld method. The triclinic structure was solved and refined in the space group $P\bar{1}$, $a = 9.377(1)$, $b = 10.113(1)$, $c = 7.138(1)$ Å, $\alpha = 97.60(1)$, $\beta = 100.88(1)$, $\gamma = 96.01(1)°$, $V = 653.0(1)$ Å^3, $Z = 2$. The structure of kingite contains finite strings of three corner sharing $Al\phi_6$ octahedra (where ϕ represents O, OH$^-$, F$^-$, or H_2O). These strings are cross-linked via PO_4 tetrahedra to produce layers that are perpendicular to [100]. The layers are linked via hydrogen bonding through H_2O located in the interlayer space. Kingite is shown to have a different stoichiometry to that reported earlier. The relationship of kingite to the structures of wavellite, $Al_3(PO_4)_2(OH)_3 \cdot 5H_2O$, and mitryaevaite, $Al_5(PO_4)_2[(P,S)O_3(OH,O)]_2F_2(OH)_2(H_2O)_8 \cdot 6.48H_2O$, are briefly discussed.